## Research Highlight Basic Energy Sciences Program Geosciences Subprogram

Title: Multi-Component Diffusion

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**Objective:** To model fingering phenomena that occur in stratified systems characterized by two of more very different diffusion coefficients for solutes and/or heat.

**Results:** We obtained good agreement between finger shapes and scales observed in Hele-Shaw laboratory experiments, and calculations based on the lattice Boltzmann (LB) method. The method has been applied to several other dispersion/reaction problems, and efficient 2D and 3D codes were developed that include buoyancy and precipitation and dissolution.

**Significance:** Double-diffusive fingering is responsible for a variety of natural phenomena. Such fingering greatly speeds mixing, and affects: the transport of materials and heat in metals casting; the evolution of stars; and the transport of solutes around salt domes, saline basins, sea-floor vents and hydrothermal systems, and contaminated soils. Perhaps the best known example of the phenomenon is "salt-fingering", which occurs when a layer of warm salt water overlies colder, fresher water as in the Mediterranean outflow. Modeling this phenomenon in the lab is difficult, since it is hard to make a "no-flux" heat boundary. The LB models developed for this project allow us to model problems beyond the scope of lab experiments, and to infer the stability limits of the phenomena.

**Publication:** Stockman, H.W.; Cooper, C.; Li, C. and Perea-Reeves, S.J. (1997) Practical application of lattice-gas and lattice Boltzmann methods to dispersion problems, *InterJournal of Complex Systems*, Article, Manuscript 90. (Electronic document available at: dyanmics.bu.edu or www.sandia.gov/eesector/gs/gc/hws/saltfing.htm.)

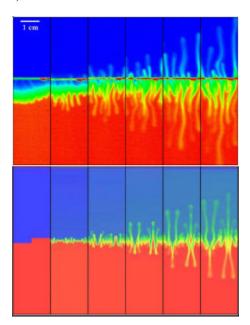


Figure 1. Top: lab Hele-Shaw experiment. Bottom: LB simulation. Red fluid is initially denser, but has higher diffusion coefficient than blue.

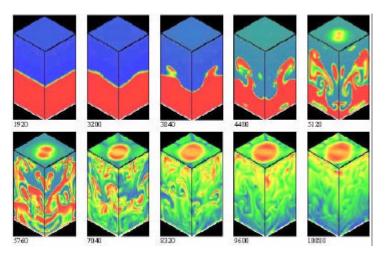


Figure 2. 3D miscible Rayleigh-Taylor instability calculation; the blue fluid is denser. Numbers are timesteps; calculation used 600,000 nodes.